

# ADAS501: SXB - graph and fit ionisation per photon coefficients

The program interrogates ionisation per photon (SXB) files of type ADF13. The coefficient is extracted for a selected radiative transition of an ion. The data may be interpolated using cubic splines at selected electron temperature/electron density pairs. A minimax polynomial approximation is made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximation.

## Background theory:

The *SXB* coefficient is the reciprocal of the *photon efficiency* coefficient. It is a convenient derived coefficient formed as a ratio of an effective ionisation rate coefficient and an effective photon emissivity coefficient. In a simple picture it relates the emission in a spectrum line integrated along a line of sight directed at a localised surface to the flux of ions from the surface.

Consider a line-of-sight orthogonal to a surface and the flux of an impurity species from the surface along the line-of-sight. Provided there is no lateral dispersion of inflowing ions from the line-of-sight or return losses to the surface, then the flux of the impurity may be obtained from an ionisation stage which ionises fully in the line-of-sight as

$$\Gamma^X = \sum_{z'=0}^z \Gamma_{z'}^X = \int_0^\infty N_e \sum_{\sigma=1}^{M_z} S_{CD,\sigma}^{(z \rightarrow z+1)} N_\sigma(\xi) d\xi \quad 6.1.1$$

where  $\xi$  is the coordinate along the line-of-sight from the surface,  $S_{CD,\sigma}^{(z \rightarrow z+1)}$  is the effective ionisation rate coefficient from the metastable  $\sigma$  of ionisation stage  $z$ . The population number density of the metastable,  $N_\sigma$ , may be obtained by observation of the emission in a spectrum line associated with the metastable ion by excitation

The emissivity in a transition  $j \rightarrow k$  of an ion may be written (see equation 3.8.7) as

$$\begin{aligned} \mathcal{E}_{j \rightarrow k} = & A_{j \rightarrow k} \left( \sum_{\sigma=1}^{M_z} \mathcal{F}_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{v'=1}^{M_{z+1}} \mathcal{F}_{jv'}^{(rec)} N_e N_{v'}^+ + \right. \\ & \left. \sum_{v'=1}^{M_{z+1}} \mathcal{F}_{jv'}^{(CX)} N_H N_{v'}^+ + \sum_{\mu'=1}^{M_{z-1}} \mathcal{F}_{j\mu'}^{(ion)} N_e N_{\mu'}^- \right) \end{aligned} \quad 6.1.2$$

$N_{v'}^+$  denotes the population density of ions in the metastable state  $v'$  of the adjacent higher ionisation stage and  $N_{\mu'}^-$  denotes the population density of ions in the metastable state  $\mu'$  of the adjacent lower ionisation stage. The  $\mathcal{F}_{j\sigma}^{(exc)}$ ,  $\mathcal{F}_{jv'}^{(rec)}$ ,  $\mathcal{F}_{jv'}^{(CX)}$  and  $\mathcal{F}_{j\mu'}^{(ion)}$  are the effective contributions to the population of the upper excited level  $j$  of the transition from excitation from the metastables, from free electron capture, from charge exchange recombination from neutral hydrogen and from ionisation respectively. All these coefficients depend on density as well as temperature.  $N_e$  is the electron density and  $N_H$  the neutral hydrogen density.

The *ionisation per photon* quantities are only meaningful for the excitation part of the emissivity. Assuming that the spectrum line  $j \rightarrow k$  may be associated solely with the metastable  $\sigma$ , then

$$N_\sigma = \mathcal{E}_{\sigma, j \rightarrow k} / N_e A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)} \quad 6.1.3$$

The flux becomes

$$\begin{aligned}
\Gamma^X &= \sum_{\sigma=1}^{M_z} \Gamma_{\sigma}^{(z)} = \int \sum_{\sigma=1}^{M_z} [S_{CD,\sigma}^{(z \rightarrow z+1)} / A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)}] \epsilon_{\sigma,j \rightarrow k}(\xi) d\xi \\
&= \sum_{\sigma=1}^{M_z} \mathcal{P}\mathcal{B}_{\sigma,j \rightarrow k} \int_0^{\infty} \epsilon_{\sigma,j \rightarrow k}(\xi) d\xi \\
&= \sum_{\sigma=1}^{M_z} \mathcal{P}\mathcal{B}_{\sigma,j \rightarrow k} I_{\sigma,j \rightarrow k}
\end{aligned}$$

6.1.4

where

$$\mathcal{P}\mathcal{B}_{\sigma,j \rightarrow k} = S_{CD,\sigma}^{(z \rightarrow z+1)} / (A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)}) = \sum_{v'=1}^{M_{z+1}} S_{CD,\sigma \rightarrow v'}^{(z \rightarrow z+1)} / (A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)})$$

6.1.5

and it is assumed that the  $\mathcal{P}\mathcal{B}$  coefficient is approximately constant over the region of emission and may be taken outside the integral.  $I_{\sigma,j \rightarrow k}$  is the line-of-sight integrated emissivity.  $S_{CD,\sigma \rightarrow v'}$  is the generalised collisional radiative coefficient from the metastable  $\sigma$  of the ion to the metastable  $v'$  of the next ionisation stage and  $S_{CD,\sigma}$  the sum over all  $v'$ . The coefficient is associated therefore with a particular spectrum line and a particular metastable of the selected ion. It depends on electron density and electron temperature in general.

#### Resolution level

A specific ion file may be specified at the LS or LSJ resolution levels. That is the populations of terms or J sub-levels are evaluated with the emissivities being correspondingly of multiplets or multiplet components. Specific ion files in ADAS for low stages of ionisation typical of inflowing species are usually of LS resolution. Nonetheless, observations at high resolution may be of individual components. Consider terms indexed by  $I$  and  $K$  with their component levels indexed by  $i$  and  $k$  so that  $i \in I$  and  $k \in K$ . It may be assumed for low stages of ionisation that the level populations of a term are relatively statistically populated. Then

$$I_{\sigma,I \rightarrow K} = \frac{w_I A_{I \rightarrow K}}{w_i A_{i \rightarrow k}} I_{\sigma,i \rightarrow k} \quad 6.1.6$$

where  $w_i$  is the statistical weight of the level  $i$  and  $w_I$  that of term  $I$ . Alternatively, if the component observations are complete,  $I_{\sigma,I \rightarrow K} = \sum_{i,k} I_{\sigma,i \rightarrow k}$  may be obtained

from experiment. The  $I_{\sigma,I \rightarrow K}$  are used with term resolved  $\mathcal{P}\mathcal{B}_{\sigma,I \rightarrow K}$  from the ADAS database.

#### Non-orthogonal line emissivities

The situation of equation 6.1.2 when a spectrum line emission depends on more than one metastable can occur and the sum over metastables must be retained for the emissivity. To obtain the fluxes in the separate metastables of the stage  $z$ , it is necessary to observe  $M_z$  line emissivities which are linearly independent. Generalising the expression

$$\epsilon_{\rho} = A_{\rho} \left( \sum_{\sigma=1}^{M_z} \mathcal{F}_{j\sigma}^{(exc)} N_e N_{\sigma} \right) \rho = 1, \dots, M_z \quad 6.1.7$$

Form the matrix  $\mathcal{P}\mathcal{B}_{\rho\sigma} = S_{CD,\sigma} / A_{\rho} \mathcal{F}_{j\sigma}$  and its inverse  $\mathcal{R} = (\mathcal{P}\mathcal{B})^{-1}$  then

$$\Gamma_{\sigma}^{(z)} = \frac{1}{\mathcal{R}_{\sigma 1}} I_1 + \frac{1}{\mathcal{R}_{\sigma 2}} I_2 + \dots + \frac{1}{\mathcal{R}_{\sigma M_z}} I_{M_z} \quad 6.1.8$$

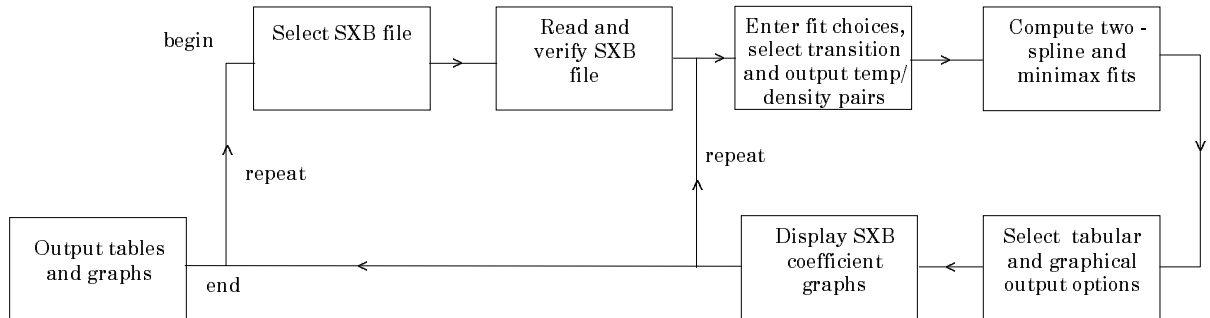
All the coefficients of the matrix  $\mathcal{P}\mathcal{B}$  are provided in the ADAS database in the metastable resolved case.

S/XB data are extracted from archived files of type ADF13. They are interpolated by cubic splines in electron temperature and density to provide results at an arbitrary set of temperature/density pairs. The interpolated data are approximated by a minimax polynomial and a graph produced. A tabulation of the the interpolated spline data and the minimax approximation is prepared.

## Program steps:

These are summarised in figure 6.1.

Figure 6.1



## Interactive parameter comments:

Programs of this series (ADAS5) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.

The **file selection window** has the appearance shown below

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size.
4. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.



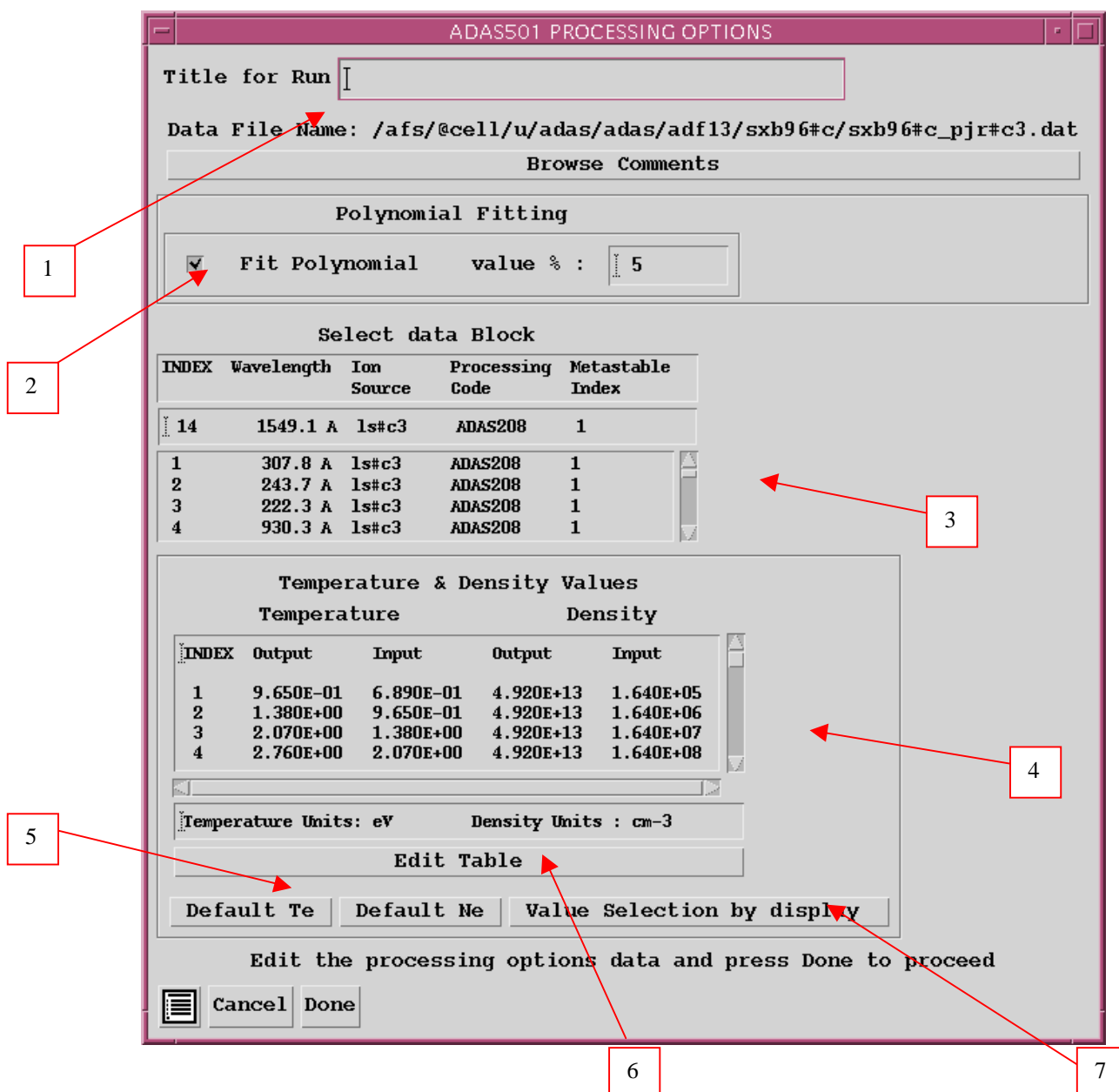
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

The **processing options window** has the appearance shown below

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted from the datafile, in the case of ADAS501, an 'emissivity coefficient', may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active.
3. Spectrum lines for which emissivity coefficients are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a line to select it. The selected line appears in the selection window just above the line list display window.
4. Your settings of electron temperature/electron density pairs (outputs) are shown in the temperature/density display window. The temperature and density values at which the emissivity coefficients are stored in the datafile (inputs) are also shown for information. **Note that you must**

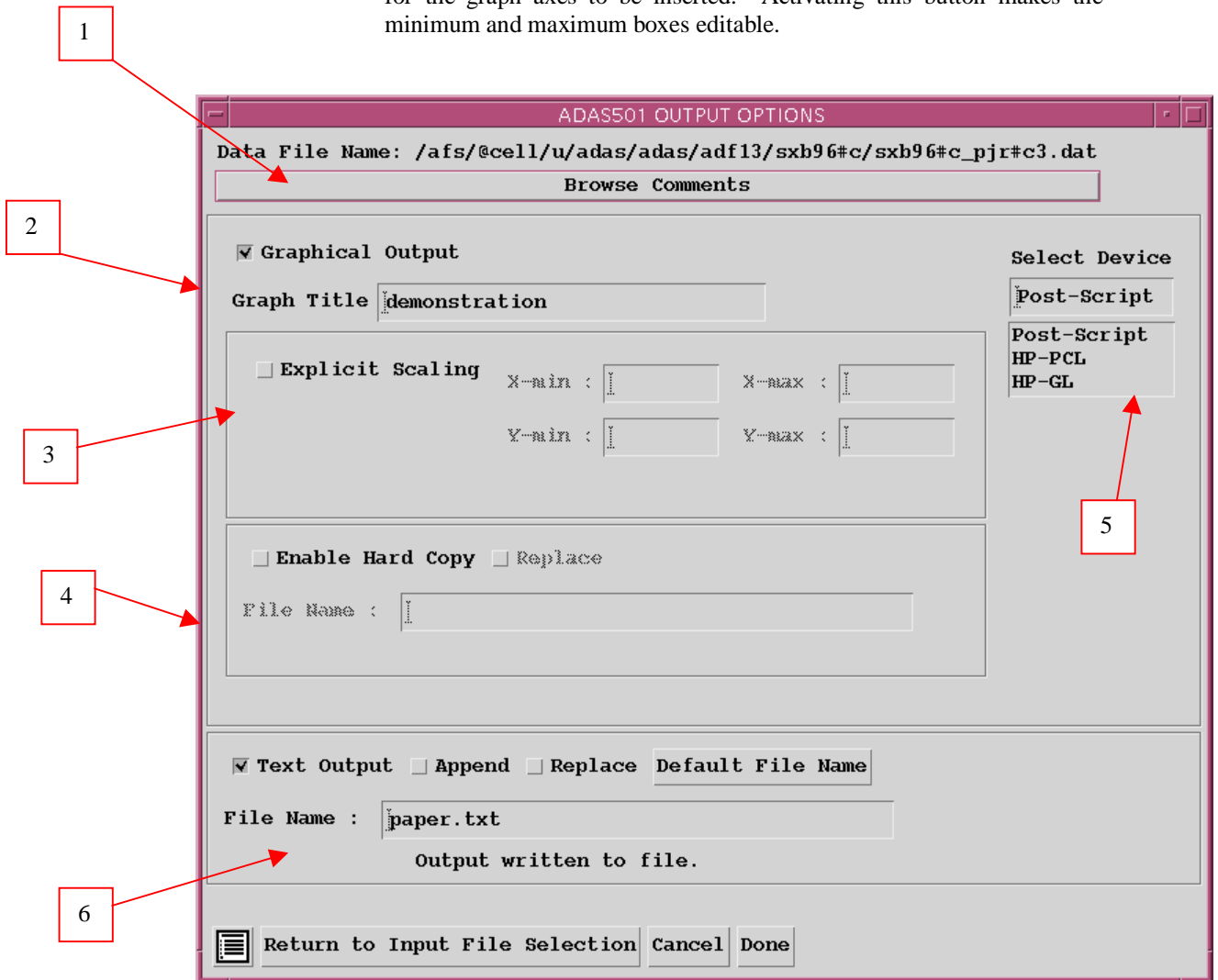
give temperature/density pairs, ie. the same number of each as for a model. The underlying datafile has a two-dimensional storage as a function of temperature and density.

5. The program recovers the output temperature/density pairs you used when last executing the program. Pressing the *Default Te* or *Default Ne* buttons insert a default set of temperatures or densities equal to the input values. A choice of particular density or particular temperature respectively from the input sets is allowed on a 'pop-up' window.
6. The Temperature & Density Values are editable. Click on the *Edit Table* button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window, appears as shown below:
7. ADAS501 has a more sophisticated graphical method for Te/Ne pair selection. Activate the *Value Selection by Display* button. The detailed operation of the widget is described in Chap1-00 of this user manual.



The output options window appearance is shown below

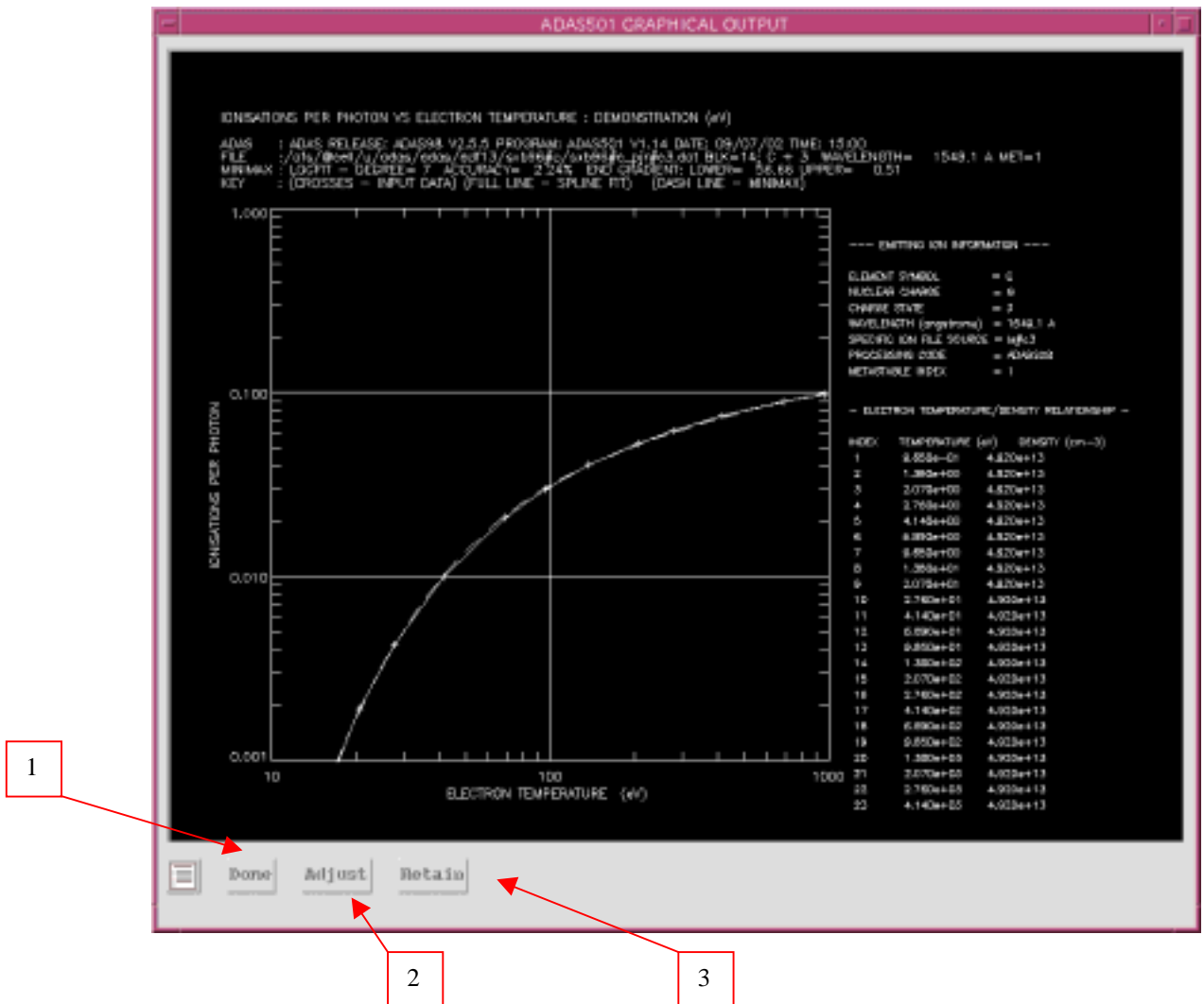
1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
3. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.



4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.
5. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
6. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
7. The graph is displayed in a following **Graphical Output** window described below.

The **Graphical output window** has some additional controls

1. Printing of the currently displayed graph is activated by the *Print* button.
2. Activate the *Adjust* button to pop-up the Graph Adjust window. Its operation is described in Chap1-00 of this user manual.
3. Activate the *Retain* button to pop-up the Multiplot window. This widget permits superposition of graphs from multiple passes through ADAS501 and hence graph comparison. The detailed operation of the widget is described in Chap1-00 of this user manual.



### Illustration:

Figure 6.3a shows a PEC coefficient of excitation type, associated with the ground state (metastable 1) for the spectrum line BeI ( $2s2p\ ^1P - 2s^2\ ^1S$ ) of neutral beryllium. The solid line connects the spline fit points obtained in the main interpolation and the dashed curve is the minimax fit.

Figure 6.1a

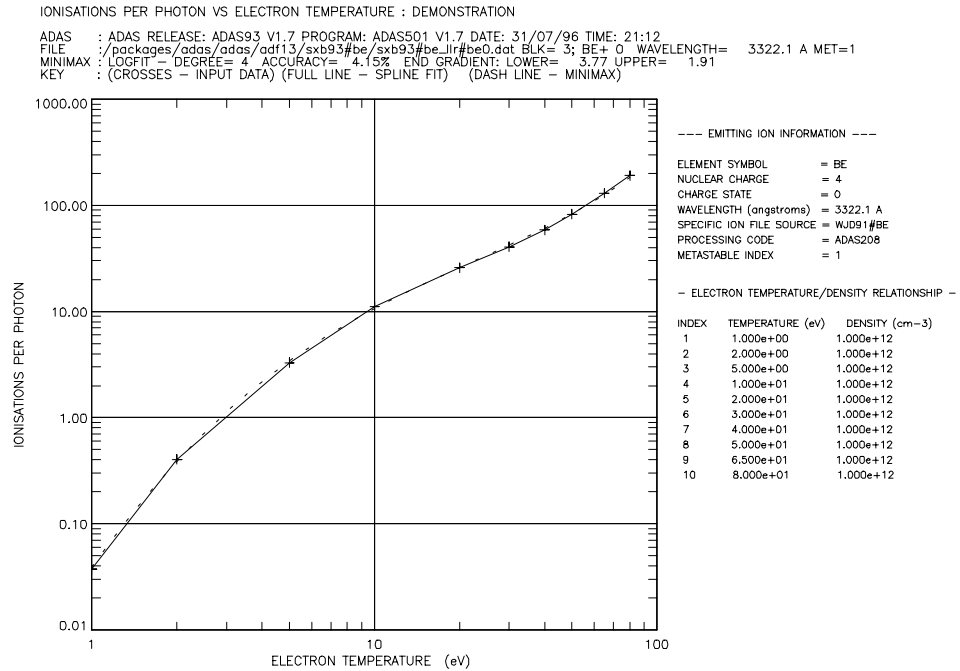


Table 6.1a

```

ADAS RELEASE: ADAS93 V1.7 PROGRAM: ADAS501 V1.7 DATE: 31/07/96 TIME: 21:12
*** TABULAR OUTPUT FROM IONIZATIONS PER PHOTON INTERROGATION PROGRAM: ADAS501 - DATE: 31/07/96
***

-----
IONIZATIONS PER PHOTON AS A FUNCTION OF ELECTRON TEMPERATURE AND DENSITY
-----

          DATA GENERATED USING PROGRAM: ADAS501
          -----
FILE : /packages/adas/adas/adf13/sxb93#be/sxb93#be_llr#be0.dat - DATA-BLOCK: 3
EMITTING ION INFORMATION:
-----
ELEMENT NAME           = BERYLLIUM
ELEMENT SYMBOL         = BE
NUCLEAR CHARGE        (Z0) = 4
CHARGE STATE          (Z) = 0
WAVELENGTH (angstroms) = 3326.1 A
SPECIFIC ION FILE SOURCE = WJD91#BE
PROCESSING CODE        = ADAS208
METASTABLE INDEX      = 1

          --- ELECTRON TEMPERATURE ---   ELECTRON DENSITY   IONIZATIONS
          kelvin          eV             cm-3             PER PHOTON
1.161D+04  1.000D+00   1.000D+12   3.730D-02
2.321D+04  2.000D+00   1.000D+12   4.040D-01
5.803D+04  5.000D+00   1.000D+12   3.280D+00
          .
          .
          .
7.544D+05  6.500D+01   1.000D+12   1.300D+02
9.284D+05  8.000D+01   1.000D+12   1.910D+02

-----
NOTE: * => IONIZATIONS PER PHOTON EXTRAPOLATED FOR TEMPERATURE/DENSITY VALUE
-----

MINIMAX POLYNOMIAL FIT TO ELECTRON TEMPERATURES - TAYLOR COEFFICIENTS:
-----
- LOG10(IONIZATIONS PER PHOTON) versus LOG10(ELECTRON TEMPERATURE<eV>) -
-----
          A( 1) = -1.410628476D+00          A( 2) = 3.767911738D+00
          A( 3) = -1.524257187D+00          A( 4) = 8.502256577D-02
          A( 5) = 1.096116453D-01
LOGFIT - DEGREE= 4 ACCURACY= 4.15% END GRADIENT: LOWER= 3.77 UPPER= 1.91
-----

```

**Notes:**